

Ensemble averaged entanglement of identical particles

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Abstract

Recent results, extending the Schmidt decomposition theorem to wavefunctions of identical particles, are reviewed. They are used to give a definition of reduced density operators in the case of two identical particles. Next, a method is discussed to calculate time averaged entanglement. It is applied to a pair of identical electrons in an otherwise empty band of the Hubbard model, and to a pair of bosons in the the Bose-Hubbard model with infinite range hopping. The effect of degeneracy of the spectrum of the Hamiltonian on the average entanglement is emphasised.

1 Introduction

Schmidt decomposition

Assume that the wavefunction $\psi(\mathbf{x}_1, \mathbf{x}_2)$ describes two distinguishable particles. Then there exist orthonormal bases of wavefunctions $\phi_m(\mathbf{x}_1)$ and $\chi_m(\mathbf{x}_2)$ and coefficients $p_m \geq 0$ such that ψ can be written as a single sum

$$\psi = \sum_m \sqrt{p_m} \phi_m \otimes \chi_m. \quad (1)$$

This result is known as the Schmidt decomposition theorem. See for instance [1], Theorem 2.7. The reduced density matrices for each of the particles are then given by

$$\sigma = \sum_m p_m |\phi_m\rangle \langle \phi_m|, \quad (2)$$

$$\tau = \sum_m p_m |\chi_m\rangle \langle \chi_m|. \quad (3)$$

Indeed, one verifies that for any one-particle operator A

$$\text{Tr } \sigma A = \sum_m p_m \langle \phi_m | A | \phi_m \rangle$$

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$$\begin{aligned}
&= \sum_m p_m \langle \phi_m \otimes \chi_m | A \otimes \mathbb{I} | \phi_m \otimes \chi_m \rangle \\
&= \langle \psi | A \otimes \mathbb{I} | \psi \rangle,
\end{aligned} \tag{4}$$

and similarly

$$\text{Tr } \tau A = \langle \psi | \mathbb{I} \otimes A | \psi \rangle. \tag{5}$$

The knowledge of the coefficients p_m suffices to calculate the von Neumann entropies

$$\mathcal{E}(\psi) = -\text{Tr } \sigma \ln \sigma = -\text{Tr } \tau \ln \tau = -\sum_m p_m \ln p_m. \tag{6}$$

The latter quantity is a measure for the entanglement of the two particles.

Identical particles

Recently [2, 3, 4], the previous result was generalised to pairs of identical particles, described by a wavefunction ψ in a Fock space. Let $b^\dagger(\phi)$ and $b(\phi)$ be the creation and annihilation operators for a particle with wavefunction $\phi(\mathbf{x})$. Let $|0\rangle$ denote the vacuum state. Then for each two-particle wavefunction ψ in a Fock space there exists an orthonormal basis of wavefunctions $\phi_m(\mathbf{x})$ in the one-particle Hilbert space and coefficients $p_m \geq 0$ such that

$$\psi = \frac{1}{\sqrt{2}} \sum_m \sqrt{p_m} b^\dagger(\phi_m) b^\dagger(\phi_m) |0\rangle, \quad (\text{bosons}) \tag{7}$$

$$\psi = \sqrt{2} \sum_m \sqrt{p_{2m}} b^\dagger(\phi_{2m}) b^\dagger(\phi_{2m+1}) |0\rangle, \quad (\text{fermions}). \tag{8}$$

If the dimension of the one-particle Hilbert space is odd then the latter expression does not involve all of the basis vectors ϕ_m .

The physical interpretation of this result, in the case of bosons, is that with probability p_m the two particles are both in the same state with wavefunction ϕ_m . In the fermionic case, one of the particles is in the state ϕ_{2m} , the other in the state ϕ_{2m+1} . It is then obvious to define reduced density matrices σ and τ by

$$\sigma = \tau = \sum_m p_m |\phi_m\rangle \langle \phi_m| \quad (\text{bosons}), \tag{9}$$

$$\sigma = 2 \sum_m p_{2m} |\phi_{2m}\rangle \langle \phi_{2m}| \quad \text{and} \quad \tau = 2 \sum_m p_{2m+1} |\phi_{2m+1}\rangle \langle \phi_{2m+1}|, \tag{10}$$

(fermions)

By convention, $p_{2n+1} = p_{2n}$ in the latter case.

In the fermion case these density matrices are far from unique since for any pair ϕ_{2m}, ϕ_{2m+1} the two basis vectors may be interchanged. Nevertheless, the resulting values of the von Neumann entropies of σ and τ are always the same. Hence, in all cases the quantity

$$\mathcal{E}(\psi) = -\sum_n p_n \ln p_n \tag{11}$$

can be used as a measure of entanglement.

In the next sections we reproduce the proofs of (9, 10) and show that the eigenvalues p_n of the reduced density matrices can be calculated without actually performing the generalised Schmidt decomposition. In this way the quantification of the entanglement of a pair of identical particles is more easy than in the case of distinguishable particles.

Linear entropy

Even the simplified method to obtain the eigenvalues p_n may be too difficult for analytical treatment. For this reason we will make use of the linear entropy instead of the von Neumann entropy (11). It is still a measure of entanglement [5], and is given by

$$\mathcal{E}_1(\psi) = \sum_n p_n(1 - p_n) = 1 - \sum_n p_n^2. \quad (12)$$

For similar reasons the von Neumann entropy has been replaced by the linear entropy in other papers as well, for instance in [6, 7, 8].

The simplification arises as follows. Let ρ be a density matrix with eigenvalues p_n . Then it is often feasible to calculate ρ^2 by matrix multiplication while the calculation of $\rho \ln \rho$ usually requires diagonalisation of ρ . Also calculating the trace of ρ^2 is usually a feasible task. The linear entropy $\mathcal{E}_1(\psi)$ is then obtained as $1 - \text{Tr} \rho^2$.

Average entanglement

A final simplification comes from averaging the linear entanglement. In principle, the entanglement of two particles depends on time. Rapid fluctuations of entanglement have been reported to occur in vibrational modes of triatomic molecules [9], and between electrons of Rydberg molecules [10]. They have been studied in theoretical models such as the Dicke model [11], a model of coupled kicked tops [12], the Harper Hamiltonian [13], a dimer model [14], Bose-Einstein condensates [15]. Hence it is obvious to study the time average of the entanglement. In [16] it is shown how to replace the time average of non-linear quantities such as the entanglement by ensemble averages. This was applied by the present authors to study the entanglement of distinguishable particles [17].

Overview of the paper

The next section recalls known results about symmetric and anti-symmetric matrices. Proofs are given in the Appendix. The theorems of [2, 3, 4] are reproduced and the calculation of the average entanglement is explained. Section 3 discusses the entanglement of a pair of identical electrons in an otherwise empty band described by the Hubbard model. Section 4 demonstrates the importance of degeneracy of the spectrum of the Hamiltonian for a two-boson model. The paper ends with a discussion in Section 5, followed by two Appendices.

2 Schmidt decomposition in Fock space

Known results on symmetric and anti-symmetric matrices

Remember that a matrix M is normal if it commutes with its hermitean conjugate M^\dagger . The transpose M^T of M has matrix elements $(M^T)_{mn} = M_{nm}$. The matrix M is symmetric if $M^T = M$, it is anti-symmetric if $M^T + M = 0$. Any matrix with complex entries M can be written as $M = V^\dagger D U$ with D diagonal and with U and V unitary. This is the singular decomposition of M . A similar result for symmetric matrices is the following theorem. It is known as Takagi's factorisation theorem – see [18], or [3], Theorem 3.4. See [19], Theorem 5.5.1, for the first claim of the theorem.

Theorem 1 *Let be given a square matrix M with complex entries. Then M is symmetric if and only if it can be written as*

$$M = U^T D U \quad (13)$$

with D diagonal and U arbitrary. The matrix U can be chosen unitary.

Consider for example the matrix M , given by

$$M = \begin{pmatrix} i & i \\ i & 1 \end{pmatrix}. \quad (14)$$

It is not normal. Still, there exists a unitary matrix U , namely

$$U = \frac{1}{2} \begin{pmatrix} 1+i & -\sqrt{2} \\ 1+i & \sqrt{2} \end{pmatrix}, \quad (15)$$

and a diagonal matrix $D = [1, 1] + (1+i)[1, -1]/\sqrt{2}$ such that $M = U^T D U$. The method to find U is based on the observation that U diagonalises $M^\dagger M$. Indeed, one has

$$M^\dagger M = U^\dagger D^\dagger D U. \quad (16)$$

This observation is essential for the calculations that follow.

The analogous result for anti-symmetric matrices is usually formulated for matrices with real entries only. For matrices with complex entries it follows from Lemma 1 of [2]. As noted in [20], the Theorem below is known in the Physics literature since long — see [21].

Theorem 2 *Let be given an anti-symmetric matrix M with complex entries. Then there exists a unitary matrix U such that M can be written as $M = U^T D U$, where D has on each row and each column at most one non-vanishing element.*

If M is anti-symmetric then also $D = (U^T)^\dagger M U^\dagger$ is anti-symmetric. Hence, if D has at most one non-vanishing element on each row and each column then it can be brought into block-diagonal form with blocks of size at most two, simply by swapping the order of rows and of columns. This is, D is a block matrix of the form

$$D = [Z_1, Z_2, \dots, Z_x, 0, 0, \dots], \quad (17)$$

with Z_j of the form

$$Z_j = \begin{pmatrix} 0 & z_1 \\ -z_1 & 0 \end{pmatrix}. \quad (18)$$

Application to wavefunctions in Fock space

Take an arbitrary orthonormal basis of wavefunctions $\omega_n(\mathbf{x})$ in a finite dimensional one-particle Hilbert space. Any two-particle wavefunction ψ can be written as

$$\psi = \sum_{mn} \lambda_{mn} \omega_m \otimes \omega_n. \quad (19)$$

The matrix of coefficients λ_{mn} is denoted Λ . In the boson case Λ is symmetric, in the fermion case it is anti-symmetric. Hence, by the previous theorems there exists a unitary matrix U and a matrix D , with at most one non-vanishing element on each row and each column, such that $\Lambda = U^T D U$. Then one can write

$$\begin{aligned} \psi &= \sum_{mnrs} U_{rm} D_{rs} U_{sn} \omega_m \otimes \omega_n \\ &= \sum_{rs} D_{rs} \phi_r \otimes \phi_s, \end{aligned} \quad (20)$$

with

$$\phi_r = \sum_m U_{rm} \omega_m. \quad (21)$$

Because the matrix D has at most one non-vanishing element on each row and each column, the double sum in (20) reduces to a single sum. This yields (7, 8, 9, 10).

Next observe that

$$\Lambda^\dagger \Lambda = (U^T D U)^\dagger U^T D U = U^\dagger D^\dagger D U. \quad (22)$$

Hence, the matrices $\Lambda^\dagger \Lambda$ and $D^\dagger D$ have the same eigenvalues. But the eigenvalues of $D^\dagger D$ are precisely the coefficients p_n appearing in the expression (11) for the entanglement. Hence, in order to calculate the entanglement of two identical systems it suffices to expand the wavefunction ψ in an arbitrary basis, as done in (19). Next, the matrix of expansion coefficients Λ is used to form $\Lambda^\dagger \Lambda$. Finally, the eigenvalues p_n of the latter matrix are calculated.

Average entanglement using the linear entropy functional

If now the linear entropy is used to quantify the entanglement instead of the von Neumann entropy then one finds

$$\mathcal{E}_1(\psi) = 1 - \text{Tr}(\Lambda^\dagger \Lambda)^2. \quad (23)$$

Next assume that the basis of eigenvectors ψ_n diagonalises the Hamiltonian H . One can expand an arbitrary wavefunction ψ in this basis

$$\psi = \sum_j \sqrt{p_n} e^{i\chi_n} \psi_n, \quad (24)$$

with real phases χ_n and positive coefficients p_n satisfying $\sum_n p_n = 1$. With each basis vector ψ_n corresponds an anti-symmetric matrix $\Lambda^{(n)}$ via (19). One then obtains

$$\mathcal{E}_1(\psi) = 1 - \sum_{mnrs} \sqrt{p_m p_n p_r p_s} e^{i(\chi_n - \chi_m)} e^{i(\chi_s - \chi_r)} \text{Tr} \Lambda^{(m)\dagger} \Lambda^{(n)} \Lambda^{(r)\dagger} \Lambda^{(s)}. \quad (25)$$

Assume now that the spectrum of H is non-degenerate. Then the time-average entanglement of ψ may be calculated as an ensemble average, by integrating over the phase factors in the above expression. The result is

$$\begin{aligned}
\overline{\mathcal{E}_1(\psi)} &= 1 - \sum_{m,r} p_m p_r \text{Tr} \Lambda^{(m)\dagger} \Lambda^{(m)} \Lambda^{(r)\dagger} \Lambda^{(r)} \\
&\quad - \sum_{m,n} p_m p_n \text{Tr} \Lambda^{(m)\dagger} \Lambda^{(n)} \Lambda^{(n)\dagger} \Lambda^{(m)} \\
&\quad + \sum_m p_m^2 \text{Tr} \left(\Lambda^{(m)\dagger} \Lambda^{(m)} \right)^2 \\
&= S_1(\sigma) + S_1(\tau) - \Delta,
\end{aligned} \tag{26}$$

with

$$\sigma = \sum_m p_m \Lambda^{(m)\dagger} \Lambda^{(m)} \tag{27}$$

$$\tau = \sum_n p_n \Lambda^{(n)} \Lambda^{(n)\dagger} \tag{28}$$

$$\Delta = 1 - \sum_m p_m^2 \text{Tr} \left(\Lambda^{(m)\dagger} \Lambda^{(m)} \right)^2. \tag{29}$$

Note that $\Lambda^{(m)\dagger} \Lambda^{(m)}$ and $\Lambda^{(m)} \Lambda^{(m)\dagger}$ have the same eigenvalues. Hence one has always $S_1(\sigma) = S_1(\tau)$.

The entanglement $\mathcal{E}_1(\psi)$ calculated above depends on the choice of the basis of eigenfunctions of the Hamiltonian. When the spectrum is non-degenerate then these eigenfunctions are unique up to a complex phase factor, which has no influence on the entanglement. Hence the problem of non-uniqueness occurs only when the spectrum is degenerate. In that case the decomposition (24) of ψ into eigenfunctions should be replaced by

$$\psi = \sum_n \sqrt{p_n} \psi'_n \tag{30}$$

with

$$\psi'_n = \frac{F_n \psi}{\|F_n \psi\|} \quad \text{and} \quad p_n = |\langle \psi_n | \psi \rangle|^2. \tag{31}$$

Here, the F_n are the orthogonal projections onto the degenerate eigenspaces of the two-particle Hamiltonian.

Examples of degeneracy are discussed below.

3 The Hubbard model

As a first application of our method we consider the average entanglement of a pair of identical electrons in an otherwise empty conduction band. A suitable description is given by the one-dimensional Hubbard model. There is an extended literature about this model. Its study accelerated after Lieb and Wu [22, 23] showed that its spectrum can be calculated using the Bethe ansatz. For

a review paper see [24]. In our treatment here both electrons have the same spin. Hence, the Hamiltonian can be simplified to

$$H = - \sum_{j,k=1}^N t_{jk} b_j^\dagger b_k, \quad (32)$$

where b_k is the annihilation operator for an electron at site k and the conjugate b_k^\dagger is the creation operator. The coefficients t_{jk} satisfy

$$t_{j,j+1} = t_{j,j-1} = 1 \quad \text{and} \quad t_{j,k} = 0 \quad \text{otherwise.} \quad (33)$$

Periodic boundary conditions are assumed, identifying site N with site 0 .

We will show that the average entanglement of the two electrons is a non-trivial conserved quantity of this model.

Entanglement of the eigenvectors

Consider a wavefunction ψ describing two identical electrons, say, both with spin up, in an otherwise empty band. Then ψ is an eigenvector of H , with eigenvalue ϵ , if and only if the anti-symmetric matrix Λ of coefficients λ_{mn} satisfies the matrix equation

$$T\Lambda + \Lambda T = -\epsilon\Lambda. \quad (34)$$

In the one-dimensional model with nearest neighbour interactions (i.e., $t_{mn} = A(\delta_{m,n+1} + \delta_{m+1,n})$ and with periodic boundary conditions (i.e., $t_{N-1,0} = t_{0,N-1} = A$) the solutions are parameterised with two integers r and s , with $r \neq s$, and are given by

$$\lambda_{mn}^{(rs)} = \frac{1}{N\sqrt{2}} [\theta(mr + ns) - \theta(nr + ms)] \quad (35)$$

with $\theta(m) = \exp(2\pi im/N)$. The corresponding eigenvalue is then

$$E^{(rs)} = -2\Re\theta(r) - 2\Re\theta(s). \quad (36)$$

Note that $\Lambda^{(rs)} = -\Lambda^{(sr)}$.

With the explicit expression (35) it is straightforward to calculate

$$\begin{aligned} \left[\Lambda^{(rs)\dagger} \Lambda^{(rs)} \right]_{mn} &= \frac{1}{2N^2} \sum_t [\overline{\theta(tr + ms)} - \overline{\theta(mr + ts)}] \\ &\quad \times [\theta(tr + ns) - \theta(nr + ts)] \\ &= \frac{1}{2N} \left[\overline{\theta(ms)}\theta(ns) + \overline{\theta(mr)}\theta(nr) \right]. \end{aligned} \quad (37)$$

Hence, one obtains

$$\begin{aligned} \text{Tr} \left[\Lambda^{(rs)\dagger} \Lambda^{(rs)} \right]^2 &= \frac{1}{4N^2} \sum_{mn} \left[\overline{\theta(ms)}\theta(ns) + \overline{\theta(mr)}\theta(nr) \right] \\ &\quad \times \left[\overline{\theta(ns)}\theta(ms) + \overline{\theta(nr)}\theta(mr) \right] \\ &= \frac{1}{2}. \end{aligned} \quad (38)$$

One concludes that all two-particle eigenvectors $\psi^{(rs)}$ are entangled, with $\mathcal{E}_1(\psi^{(rs)}) = 1/2$.

One can do even more. The vectors u^\pm with components

$$u_m^\pm = \overline{\theta(mr)} \pm \overline{\theta(ms)} \quad (39)$$

are eigenvectors of the matrix $\Lambda^{(rs)\dagger} \Lambda^{(rs)}$ with eigenvalue 1/2. All other eigenvectors have eigenvalue 0. Hence, with the notations of previous sections the only non-vanishing eigenvalues are $p_0 = p_1 = 1/2$. The entanglement of the two-particle eigenvectors $\psi^{(rs)}$, using the von Neumann entropy, is therefore

$$\mathcal{E}(\psi^{(rs)}) = 2\left(-\frac{1}{2} \ln \frac{1}{2}\right) = \ln 2. \quad (40)$$

Average entanglement

Let us now calculate the average entanglement of an arbitrary two-particle wavefunction. One has

$$\Delta = 1 - \frac{1}{2} \sum_{rs} p_{rs}^2. \quad (41)$$

Similarly is

$$\begin{aligned} \text{Tr} \left[\Lambda^{(rs)\dagger} \Lambda^{(rs)} \right] \left[\Lambda^{(r's')\dagger} \Lambda^{(r's')} \right] &= \frac{1}{4N^2} \sum_{mn} \left[\overline{\theta(ms)} \theta(ns) + \overline{\theta(mr)} \theta(nr) \right] \\ &\quad \times \left[\overline{\theta(ns')} \theta(ms') + \overline{\theta(nr')} \theta(mr') \right] \\ &= \frac{1}{4} [\delta_{ss'} + \delta_{rr'} + \delta_{rs'} + \delta_{sr'}]. \end{aligned} \quad (42)$$

Hence

$$S(\sigma) = S(\tau) = 1 - \frac{1}{4} \sum_{rr'ss'} p_{rs} p_{r's'} [\delta_{ss'} + \delta_{rr'} + \delta_{rs'} + \delta_{sr'}]. \quad (43)$$

Using (26) and the normalisation condition

$$\sum_{r>s} p_{rs} = 1 \quad (44)$$

one calculates

$$\begin{aligned} \overline{\mathcal{E}_1(\psi)} &= \frac{1}{2} + \frac{1}{2} \left[\sum_{r>s} p_{rs} \right]^2 + \frac{1}{2} \sum_{rs} p_{rs}^2 \\ &\quad - \frac{1}{2} \sum_{rr'ss'} p_{rs} p_{r's'} [\delta_{ss'} + \delta_{rr'} + \delta_{rs'} + \delta_{sr'}] \\ &= \frac{1}{2} + \sum'_{rr'ss'} p_{rs} p_{r's'}, \end{aligned} \quad (45)$$

where the summation \sum' is restricted to the sets of indices $rr'ss'$ satisfying $r > r'$, $s > s'$, $r \neq s$, $r \neq s'$, $r' \neq s$, $r' \neq s'$.

In the above calculation the degeneracy of the spectrum has been neglected. As a consequence, the result is only valid when the projection of ψ on any of the degenerate subspaces is always parallel to one of the basis vectors $\psi^{(rs)}$. This is not the case in general. The calculation of the entanglement of an arbitrary wavefunction is therefore more complicated. We will not treat this general case but end this section with an example where degeneracy does not play. The complications due to degeneracy will be discussed in the bosonic example of the next section.

Example with $N = 4$

Take $N = 4$. This means that the two electrons occupy 4 sites on a ring. The eigenvalues are -2,0,2, each twofold degenerate. The corresponding eigenvectors are $\psi^{(1,4)}$ and $\psi^{(3,4)}$, $\psi^{(1,3)}$ and $\psi^{(2,4)}$, and $\psi^{(1,2)}$ and $\psi^{(2,3)}$. We neglect the effect of the degeneracy on the average entanglement with the argument that it can be lifted by adding a small perturbation to the model.

Let

$$\psi = \sqrt{p}\psi^{(1,4)} + \sqrt{1-p}\psi^{(2,3)}. \quad (46)$$

Projection of ψ onto the eigenspace with eigenvalue -2 gives the former term, onto the eigenspace with eigenvalue +2 the latter term. The average linear entanglement is

$$\begin{aligned} \overline{\mathcal{E}_1(\psi)} &= \frac{1}{2} + p_{1,4}p_{2,3} \\ &= 1/2 + p(1-p). \end{aligned} \quad (47)$$

4 The bosonic model

As an example of the bosonic case we consider a model which is similar to the boson-Hubbard model [25, 26, 27].

The bosonic creation and annihilation operators satisfy the commutation relations $[b_j, b_k^\dagger] = \delta_{jk}$. The Hamiltonian is given by

$$H = + \sum_{j,k=1}^N t_{jk} b_j^\dagger b_k. \quad (48)$$

However, unlike in the boson-Hubbard model, the hopping coefficients are not restricted to nearest neighbour. They rather satisfy

$$t_{jk} = [1 - (N-1)\epsilon]\delta_{jk} + \epsilon(1 - \delta_{jk}). \quad (49)$$

This model is known as the Bose-Hubbard model with infinite range hopping [28].

Degeneracy is very important in this model. Indeed, assume $\epsilon > 0$. Then the ground state of the one-particle Hamiltonian is $N - 1$ -fold degenerate. Hence, the two-particle system has only three energy levels. We will consider the state $|1, 1, 0, 0, \dots, 0\rangle$, in which the photons are not entangled. Next we calculate the average entanglement and show that it tends to 1/2 when the size N of the system becomes large.

Projection onto invariant subspaces

The one-particle ground state is $N - 1$ -fold degenerate with energy $1 - N\epsilon$. Indeed, one calculates for $m \neq n$

$$\begin{aligned} H(b_m^\dagger - b_n^\dagger)|0\rangle &= \sum_j (t_{jm} - t_{jn})b_j^\dagger|0\rangle \\ &= (1 - N\epsilon)(b_m^\dagger - b_n^\dagger)|0\rangle. \end{aligned} \quad (50)$$

$N - 1$ of these vectors $(b_m^\dagger - b_n^\dagger)|0\rangle$ are linearly independent. The remaining eigenstate, orthogonal to the ground states, has eigenvalue 1. Its wavefunction is

$$\frac{1}{\sqrt{N}} \sum_{j=1}^N b_j^\dagger|0\rangle = b^\dagger(\phi^{(0)})|0\rangle, \quad (51)$$

with

$$\phi^{(0)} = \frac{1}{\sqrt{N}} \sum_j \omega_j \quad (52)$$

and ω_j the one-particle basis formed by $\omega_j = b_j^\dagger|0\rangle$. Each of these basis vectors can be projected onto this eigenvector

$$\omega_j = \frac{1}{\sqrt{N}} \phi^{(0)} + \xi_j. \quad (53)$$

The vectors ξ_j are orthogonal to $\phi^{(0)}$ and hence belong to the degenerate space of eigenvectors.

The one-particle eigenfunction ψ_0 determines an eigenstate $\psi^{(00)}$ of the two-particle Hamiltonian by

$$\psi^{(00)} = \frac{1}{\sqrt{2}} b^\dagger(\phi^{(0)}) b^\dagger(\phi^{(0)})|0\rangle. \quad (54)$$

The initial state

$$\psi = |1, 1, 0, 0, \dots\rangle = b_1^\dagger b_2^\dagger|0\rangle \quad (55)$$

is now projected onto the three invariant subspaces by writing it into the form

$$\begin{aligned} |1, 1, 0, 0, \dots\rangle &= \frac{1}{N} b^\dagger(\phi^{(0)}) b^\dagger(\phi^{(0)})|0\rangle \\ &\quad + \frac{1}{\sqrt{N}} b^\dagger(\phi^{(0)}) b^\dagger(\xi_1 + \xi_2)|0\rangle \\ &\quad + b^\dagger(\xi_1) b^\dagger(\xi_2)|0\rangle \\ &\equiv \sqrt{p^{(00)}} \psi^{(00)} + \sqrt{p^{(11)}} \psi^{(11)} + \sqrt{p^{(01)}} \psi^{(01)}, \end{aligned} \quad (56)$$

with normalised eigenfunctions $\psi^{(\sigma, \tau)}$ and normalisation constants $p^{(\sigma, \tau)}$. It is straightforward to find that (see the Appendix B)

$$p^{(00)} = \frac{2}{N^2}, \quad p^{(11)} = \left(1 - \frac{1}{N}\right)^2 + \frac{1}{N^2}, \quad p^{(01)} = \frac{2}{N} \left(1 - \frac{2}{N}\right). \quad (57)$$

Entanglement

Next, one should decompose the eigenfunctions $\psi^{(00)}, \psi^{(11)}, \psi^{(01)}$ into the basis vectors

$$\psi^{(\sigma,\tau)} = \sum_{jk} \lambda_{jk}^{(\sigma,\tau)} \omega_j \otimes \omega_k. \quad (58)$$

The calculation of the matrices $\Lambda^{(00)}, \Lambda^{(11)}, \Lambda^{(01)}$ is found in the Appendix B. — see (80, 81, 82). These are used to calculate the density matrices σ, τ , and the average entanglements

$$\mathcal{E}(\sigma) = \mathcal{E}(\tau) = \frac{1}{2} + \frac{1}{N} - \frac{2}{N^2}. \quad (59)$$

and

$$\Delta = \frac{1}{2} + \frac{2}{N} - \frac{8}{N^2} + \frac{16}{N^3} - \frac{16}{N^4}. \quad (60)$$

See the Appendix B. The final result is

$$\overline{\mathcal{E}_1(\psi)} = \frac{1}{2} + \frac{4}{N^2} \left(1 - \frac{2}{N}\right)^2. \quad (61)$$

The average entanglement is always larger than $1/2$, is maximal at $N = 4$ with a value of $9/16$, and converges as $1/N^2$ towards $1/2$ for large N .

5 Discussion

In a rather long Introduction we have summed up a number of results that appeared in the literature. We have reviewed known properties of symmetric and anti-symmetric matrices, with proofs in the Appendix A. When applied to wavefunctions in a Fock space they lead to the definition of reduced density operators for systems consisting of two identical particles. These results are known. They generalise the Schmidt decomposition theorem to pairs of identical particles. We propose to take this generalised decomposition theorem as the basis for defining a measure of entanglement of two identical particles. Up to now, many authors have used for identical particles the same expressions as for distinguishable particles. This leads to the artificial result that the entanglement of two identical fermions is always larger than 1. Subtracting this constant 1 is not needed when using the definition (6).

In Section 3, the technique to calculate the time-averaged entanglement is explained. The linear entropy is used instead of the von Neumann entropy in order to simplify the calculations. The extension of this technique to systems of two identical particles is straightforward, using the generalised Schmidt decomposition.

Two applications have been considered, one for fermions, the other for bosons. In the Hubbard model the average entanglement of two identical electrons can be calculated for arbitrary initial conditions. However, in this calculation we have neglected the effect of degeneracy of the spectrum of the Hamiltonian. This can be justified with the argument that small perturbations caused

by the environment would lift the degeneracy. The average entanglement obtained in this way is always larger than one half and is a non-trivial conserved quantity. In the boson model the degeneracy is much worse, leaving only three distinct energy levels. For one particular initial state we have shown that the average entanglement can be calculated, taking degeneracy into account. The resulting value tends to $1/2$ when the size of the system becomes large.

Related results have been obtained by other authors. Lévy et al [20] consider 2 fermions in combination with a one-particle Hilbert space of dimension 4. Wang and Sanders [29] use the generalised decomposition theorem to decompose the state of the system into qubit states. Next they calculate the entanglement of one qubit with the others and average over the choice of qubits.

Only bipartite entanglement has been considered in the present paper. Multipartite entanglement is more complicated and requires additional investigation. See for instance [30, 31, 32]. Neither did we study spatial entanglement of identical particles [33, 34, 35], or other measures of entanglement, like concurrence [35]. Finally, note that we assume that the time evolution is unitary. One expects that, due to interactions with the environment, entanglement will fade away. See the review paper [36].

Appendix A

For the sake of completeness, we give here a proof of Theorems 1 and 2. First assume normal matrices.

Proposition 1 *If M is normal and symmetric then there exists an orthogonal matrix V and a diagonal matrix D such that $M = V^T D V$.*

Proof

Let $\{E^{(n)}\}_n$ be a spectral family in a finite dimensional Hilbert space. Then there exists a unitary matrix V and two-by-two disjoint sets I_n such that

$$E^{(n)} = V^\dagger \mathbb{I}^{(n)} V \quad (62)$$

where

$$\begin{aligned} \mathbb{I}_{pq}^{(n)} &= 1 && \text{if } p = q \in I_n \\ &= 0 && \text{otherwise.} \end{aligned} \quad (63)$$

Note that

$$E_{pq}^{(n)} = \sum_{r \in I_n} \overline{V_{rp}} V_{rq}. \quad (64)$$

Hence, if $E^{(n)}$ is symmetric then all elements $E_{pq}^{(n)}$ are real. This implies that, if all $E^{(n)}$ are symmetric, then V can be chosen orthogonal, i.e. $V^\dagger = V^T$.

Let $M = \sum_n \lambda_n E^{(n)}$ be the spectral decomposition of M with all λ_n two by two distinct. Then also the $E^{(n)}$ are symmetric because of the uniqueness of the spectral decomposition and because the transpose of an orthogonal projection

operator is again an orthogonal projection operator. Hence there exists an orthogonal matrix V such that

$$M = V^T D V \quad \text{with} \quad D = \sum_n \lambda_n \mathbb{I}^{(n)}. \quad (65)$$

□

If M is anti-symmetric then

$$0 = \sum_n \lambda_n \left[E^{(n)} + (E^{(n)})^T \right]. \quad (66)$$

This does not imply that the $E^{(n)}$ are anti-symmetric (which is impossible for a non-vanishing orthogonal projection operator anyway)! Hence a different line of reasoning is needed.

Proposition 2 *If M is normal and anti-symmetric then there exists a unitary matrix U such that $U^T M U$ has on each row and each column at most one non-vanishing element.*

Proof

Let $M = \sum_n \lambda_n E^{(n)}$ be the spectral decomposition of M with all λ_n two by two distinct. Now assume ζ is an eigenvector of M with eigenvalue $\lambda_n \neq 0$, satisfying $E^{(n)} \zeta = \zeta$. Define η by $\eta_r = \overline{\zeta_r}$. Then one has

$$\begin{aligned} (M\eta)_r &= \sum_s M_{rs} \eta_s \\ &= - \sum_s M_{sr} \overline{\zeta_s} \\ &= - \overline{\sum_s (M^\dagger)_{rs} \zeta_s} \\ &= - \overline{(M^\dagger \zeta)_r} \\ &= -\lambda_n \eta_r. \end{aligned} \quad (67)$$

Hence, η is an eigenvector of M with eigenvalue $-\lambda_n$. This implies that either $\lambda_n = 0$ or there exists $m \neq n$ such that $\lambda_m = -\lambda_n$. In the latter case, m and n are matching indices and $E^{(m)}$ projects on all vectors η obtained by taking elementwise complex conjugation of all vectors in the range of $E^{(n)}$.

Now choose an orthonormal basis $\zeta^{(1)}, \zeta^{(2)}, \dots, \zeta^{(q)}$ in the range of $E^{(n)}$ and a corresponding basis $\eta^{(1)}, \eta^{(2)}, \dots, \eta^{(q)}$ in the range of $E^{(m)}$, with $\eta_s^{(j)} = \overline{\zeta_s^{(j)}}$. Do this for all non-vanishing pairs of eigenvalues $\lambda_m = -\lambda_n$. Complement this with an orthonormal basis in the nullspace of M , if present. Collect all these basis vectors as columns of a unitary matrix U . For a given $\zeta^{(j)}$ in the range of $E^{(n)}$ is, with some abuse of notation,

$$(U^T M U \delta_j)_p = (U^T M U)_{rj}$$

$$\begin{aligned}
&= \sum_s (U^T M)_{rs} \zeta_s^{(j)} \\
&= \lambda_j \sum_s (U^T)_{rs} \zeta_s^{(j)} \\
&= \lambda_j \sum_s \zeta_s^{(r)} \zeta_s^{(j)} \\
&= \lambda_j \langle \eta^{(r)} | \zeta^{(j)} \rangle.
\end{aligned} \tag{68}$$

By construction, the latter vanishes for all but at most one value of r . This ends the proof. \square

Finally, the above results are generalised to arbitrary square matrices. The argument is that found in the proof of [2], Lemma 1.

Let be given a matrix M which is either symmetric or anti-symmetric. The matrix MM^\dagger is hermitean and can be diagonalised by means of a unitary matrix U , i.e. $U^\dagger MM^\dagger U$ is diagonal. Let $C = U^\dagger M (U^\dagger)^T$. Then C , like M , is either symmetric or anti-symmetric. In addition it satisfies (using that $U^\dagger MM^\dagger U$ is diagonal and that $M^T = \pm M$)

$$CC^\dagger = U^\dagger MM^\dagger U = (U^\dagger MM^\dagger U)^T = U^T M^\dagger M (U^T)^\dagger = C^\dagger C. \tag{69}$$

This means that C is normal and that, by the previous propositions, there exists a unitary matrix V such that $V^T C V$ has on each row and each column at most one non-vanishing element. The proof of the two theorems then follows easily.

Appendix B

Here we present the calculation of the time average entanglement of the initial boson state

$$\psi = |1, 1, 0, \dots, 0\rangle = b_1^\dagger b_2^\dagger |0\rangle. \tag{70}$$

See Section 4.

The non-degenerate eigenvector of the two-particle Hamiltonian is

$$\psi^{(00)} = \frac{1}{\sqrt{2}} b^\dagger(\phi^{(0)}) b^\dagger(\phi^{(0)}) |0\rangle = \frac{1}{N\sqrt{2}} \sum_{j,k} b_j^\dagger b_k^\dagger |0\rangle \tag{71}$$

It has eigenvalue 2. The projection of $|1, 1, 0, 0, \dots\rangle$ onto this eigenvector is $\sqrt{p^{(00)}} \psi^{(00)}$ with $p^{(00)} = 2/N^2$.

Introduce vectors ξ_j , orthogonal to $\phi^{(0)}$, determined by

$$\omega_j = \langle \phi^{(0)} | \omega_j \rangle \phi^{(0)} + \xi_j = \frac{1}{\sqrt{N}} \phi^{(0)} + \xi_j. \tag{72}$$

Then one can write

$$\begin{aligned}
|1, 1, 0, 0, \dots\rangle &= \frac{1}{N} b^\dagger(\phi^{(0)}) b^\dagger(\phi^{(0)}) |0\rangle + b^\dagger(\xi_1) b^\dagger(\xi_2) |0\rangle \\
&\quad + \frac{1}{\sqrt{N}} b^\dagger(\phi^{(0)}) b^\dagger(\xi_1 + \xi_2) |0\rangle.
\end{aligned} \tag{73}$$

The projection of $|1, 1, 0, 0, \dots\rangle$ onto the $(N-1)^2$ -fold degenerate subspace equals $b^\dagger(\xi_1)b^\dagger(\xi_2)|0\rangle$. It is written as $\sqrt{p^{(11)}}\psi^{(11)}$ with

$$\begin{aligned} p^{(11)} &= ||b^\dagger(\xi_1)b^\dagger(\xi_2)|0\rangle||^2 \\ &= \langle\xi_1|\xi_1\rangle\langle\xi_2|\xi_2\rangle + |\langle\xi_1|\xi_2\rangle|^2 \\ &= \left(1 - \frac{1}{N}\right)^2 + \frac{1}{N^2}. \end{aligned} \quad (74)$$

The projection of $|1, 1, 0, 0, \dots\rangle$ onto the remaining subspace equals

$$\frac{1}{\sqrt{N}}b^\dagger(\phi^{(0)})b^\dagger(\xi_1 + \xi_2)|0\rangle. \quad (75)$$

It is written as $\sqrt{p^{(01)}}\psi^{(01)}$ with

$$\begin{aligned} p^{(01)} &= \frac{1}{N}||b^\dagger(\phi^{(0)})b^\dagger(\xi_1 + \xi_2)|0\rangle||^2 \\ &= \frac{1}{N}||\xi_1 + \xi_2||^2 \\ &= \frac{2}{N}\left(1 - \frac{2}{N}\right). \end{aligned} \quad (76)$$

Explicit expressions for the three eigenstates are

$$\begin{aligned} \psi^{(00)} &= \phi^{(0)} \otimes \phi^{(0)} \\ &= \frac{1}{N} \sum_{jk} \omega_j \otimes \omega_k, \end{aligned} \quad (77)$$

$$\begin{aligned} \psi^{(11)} &= \frac{1}{\sqrt{p^{(11)}}} \frac{1}{\sqrt{2}} (\xi_1 \otimes \xi_2 + \xi_2 \otimes \xi_1) \\ &= \frac{1}{\sqrt{p^{(11)}}} \frac{1}{\sqrt{2}} \left[\omega_1 \otimes \omega_2 + \omega_2 \otimes \omega_1 + \frac{2}{N} \phi^{(0)} \otimes \phi^{(0)} \right. \\ &\quad \left. - \frac{1}{\sqrt{N}} \phi^{(0)} \otimes \omega_1 - \frac{1}{\sqrt{N}} \omega_1 \otimes \phi^{(0)} \right. \\ &\quad \left. - \frac{1}{\sqrt{N}} \phi^{(0)} \otimes \omega_2 - \frac{1}{\sqrt{N}} \omega_2 \otimes \phi^{(0)} \right], \end{aligned} \quad (78)$$

$$\begin{aligned} \psi^{(01)} &= \frac{1}{\sqrt{p^{(01)}}} \frac{1}{\sqrt{2N}} \left(\phi^{(0)} \otimes (\xi_1 + \xi_2) + (\xi_1 + \xi_2) \otimes \phi^{(0)} \right) \\ &= \frac{1}{\sqrt{p^{(01)}}} \frac{1}{\sqrt{2N}} \left[\phi^{(0)} \otimes (\omega_1 + \omega_2) + (\omega_1 + \omega_2) \otimes \phi^{(0)} \right. \\ &\quad \left. - \frac{4}{\sqrt{N}} \phi^{(0)} \otimes \phi^{(0)} \right]. \end{aligned} \quad (79)$$

The coefficients of the expansion of each of the vectors $\psi^{(00)}$, $\psi^{(11)}$, and $\psi^{(01)}$ into the basis vectors $\omega_j \otimes \omega_k$ can be written as

$$\lambda_{jk}^{(00)} = \frac{1}{2} x_{jk}^{(1)}, \quad (80)$$

$$\lambda_{jk}^{(11)} = \frac{1}{\sqrt{p^{(11)}}} \frac{1}{2N\sqrt{2}} \left[2x_{jk}^{(1)} - 2x_{jk}^{(3)} + Nx_{jk}^{(2)} - Ny_{jk} \right], \quad (81)$$

$$\lambda_{jk}^{(01)} = \frac{1}{\sqrt{p^{(01)}}} \frac{1}{N\sqrt{2}} \left[x_{jk}^{(3)} - 2x_{jk}^{(1)} \right], \quad (82)$$

with

$$x_{jk}^{(1)} = \frac{2}{N}, \quad (83)$$

$$x_{jk}^{(2)} = (\delta_{j1} + \delta_{j2})(\delta_{k1} + \delta_{k2}), \quad (84)$$

$$x_{jk}^{(3)} = \delta_{j1} + \delta_{k1} + \delta_{j2} + \delta_{k2}, \quad (85)$$

$$y_{jk} = (\delta_{j1} - \delta_{j2})(\delta_{k1} - \delta_{k2}). \quad (86)$$

The matrices $X^{(1)}$, $X^{(2)}$, $X^{(3)}$ span a simple Jordan algebra of the spin factor type (see [37], Section 2.9.7). The Jordan product is defined by

$$A * B = \frac{1}{2}(AB + BA). \quad (87)$$

One verifies that

$$X^{(1)} * X^{(1)} = 2X^{(1)} \quad (88)$$

$$X^{(2)} * X^{(2)} = 2X^{(2)} \quad (89)$$

$$X^{(3)} * X^{(3)} = 2X^{(3)} + NX^{(2)} + NX^{(1)} \quad (90)$$

$$X^{(1)} * X^{(2)} = \frac{2}{N}X^{(3)} \quad (91)$$

$$X^{(1)} * X^{(3)} = 2X^{(1)} + X^{(3)} \quad (92)$$

$$X^{(2)} * X^{(3)} = X^{(3)} + 2X^{(2)} \quad (93)$$

$$Y * Y = 2Y \quad (94)$$

$$Y * X^{(j)} = 0, \quad j = 1, 2, 3. \quad (95)$$

There exists a representation of the Jordan algebra with the above product rules in $\mathbb{R}^2 + \mathbb{R} + \mathbb{R}$, with the product rule

$$(u, a, \lambda) * (v, b, \mu) = (av + bu, \langle u|v \rangle + ab, \lambda\mu). \quad (96)$$

Let $u^{(1)}$ and $u^{(2)}$ be two unit vectors satisfying $\langle u^{(1)}|u^{(2)} \rangle = -1 + 4/N$. Then one can identify

$$X^{(1)} = (u^{(1)}, 1, 0) \quad (97)$$

$$X^{(2)} = (u^{(2)}, 1, 0) \quad (98)$$

$$X^{(3)} = \frac{1}{2}(N(u^{(1)} + u^{(2)}), 4, 0) \quad (99)$$

$$Y = (0, 0, 2). \quad (100)$$

With this representation is

$$\sqrt{p^{(00)}}\Lambda^{(00)} = \frac{1}{N\sqrt{2}}(u^{(1)}, 1, 0) \quad (101)$$

$$\begin{aligned} \sqrt{p^{(11)}}\Lambda^{(11)} &= \frac{1}{2N\sqrt{2}}[2X^{(1)} - 2X^{(3)} + NX^{(2)} - NY] \\ &= \frac{1}{2N\sqrt{2}}(-(N-2)u^{(1)}, N-2, -2N) \end{aligned} \quad (102)$$

$$\sqrt{p^{(01)}}\Lambda^{(01)} = \frac{1}{N\sqrt{2}}[X^{(3)} - 2X^{(1)}]$$

$$= \frac{1}{2N\sqrt{2}}((N-4)u^{(1)} + Nu^{(2)}, 0, 0). \quad (103)$$

It is now straightforward to calculate the squares

$$p^{(00)}(\Lambda^{(00)})^2 = \frac{1}{N^2}(u^{(1)}, 1, 0) \quad (104)$$

$$p^{(11)}(\Lambda^{(11)})^2 = \frac{1}{4N^2}(-(N-2)^2u^{(1)}, (N-2)^2, 2N^2) \quad (105)$$

$$p^{(01)}(\Lambda^{(01)})^2 = \frac{1}{N^2}(0, N-2, 0). \quad (106)$$

Summing these relations gives

$$\sigma = \tau = \frac{1}{4N}(-(N-4)u^{(1)}, N, 2N). \quad (107)$$

Squaring again gives

$$\sigma^2 = \tau^2 = \frac{1}{16N^2}(-2N(N-4)u^{(1)}, N^2 + (N-4)^2, 4N^2). \quad (108)$$

The trace of the matrix represented by (u, a, λ) equals $2a + \lambda$. Hence, one finds (59).

Let us finally calculate Δ . Squaring again gives

$$\left(p^{(00)}(\Lambda^{(00)})^2\right)^2 = \frac{2}{N^4}(u^{(1)}, 1, 0) \quad (109)$$

$$\left(p^{(11)}(\Lambda^{(11)})^2\right)^2 = \frac{1}{8N^4}(-(N-2)^4u^{(1)}, (N-2)^4, 2N^4) \quad (110)$$

$$\left(p^{(01)}(\Lambda^{(01)})^2\right)^2 = \frac{1}{N^4}(0, (N-2)^2, 0). \quad (111)$$

This gives

$$\begin{aligned} \Delta &= 1 - \text{Tr} \left(p^{(00)}(\Lambda^{(00)})^2\right)^2 - \text{Tr} \left(p^{(11)}(\Lambda^{(11)})^2\right)^2 - \text{Tr} \left(p^{(01)}(\Lambda^{(01)})^2\right)^2 \\ &= \frac{1}{2} + \frac{2}{N} - \frac{8}{N^2} + \frac{16}{N^3} - \frac{16}{N^4}. \end{aligned} \quad (112)$$

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